

1-Hexanol
111-27-3 | DTXSID8021931

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 151 °C

Global applicability domain: Inside

Local applicability domain index: 8.70e-01

Confidence level: 8.53e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1-Hexanol

Measured: 158

Predicted: 151

[Image not found](#)

4-Methylpentan-1-ol

Measured: 152

Predicted: 147

[Image not found](#)

2-Methyl-1-pentanol

Measured: 149

Predicted: 145

[Image not found](#)

2-Ethyl-1-butanol

Measured: 147

Predicted: 144